ANL/MSD/CP--93077

CONF-970834--28

RECEIVED

AUG 12 1997

OSTI

ATOMIC STRUCTURE OF [110] TILT GRAIN
BOUNDARIES IN FCC MATERIALS*

K. L. Merkle and L. J. Thompson

*Materials Science Division
Argonne National Laboratory
Argonne, IL 60439*

April 1997

The submitted manuscript has been created by the University of Chicago as Operator of Argonne National Laboratory ("Argonne") under Contract No. W-31-109-ENG-38 with the U.S. Department of Energy. The U.S. Government retains for itself, and others acting on its behalf, a paid-up, non exclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to and display publicly, by or on behalf of the Government.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Invited paper to be submitted to Microscopy and Microanalysis, August 10-14, 1997, Cleveland, OH.

*Work supported by the U.S. Department of Energy, Basic Energy Sciences-Materials Sciences, grant No. W-31-109-ENG-38.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ATOMIC STRUCTURE OF [110] TILT GRAIN BOUNDARIES IN FCC MATERIALS

K. L. Merkle and L. J. Thompson

Materials Science Division, Argonne National Laboratory, Argonne, IL 60439

High-resolution electron microscopy (HREM) has been used to study the atomic-scale structure and localized relaxations at grain boundaries (GBs) in Au, Al, and MgO. The [110] tilt GBs play an important role in polycrystalline fcc metals since among all of the possible GB geometries this series of misorientations as a whole contains the lowest energies, including among others the two lowest energy GBs, the (111) and (113) twins.¹ Therefore, studies of the atomic-scale structure of [110] tilt GBs in fcc metals and systematic investigations of their dependence on misorientation and GB plane is of considerable importance to materials science. [110] tilt GBs in ceramic oxides of the fcc structure are also of considerable interest, since in this misorientation range polar GBs exist, i. e. GBs in which crystallographic planes that are made up of complete layers of cations or anions can join to form a GB.

Thin singlecrystalline films of (110) Au were prepared by vacuum evaporation of Au onto (110) NaCl. Au tilt GBs were obtained by welding two epitaxially grown films at the desired misorientation angle and converting twist to tilt GBs by a suitable annealing treatment that changed the orientation of the GB plane from the twist to tilt configuration. Al and MgO bicrystal samples were obtained by templating onto Au films containing tilt GBs. Suitably thin samples for HREM observation were obtained by ion milling. The samples typically contained many [110] tilt GBs, mostly in the form of island grains of various sizes. We could therefore study the role of the GB plane at a given misorientation, since in principle all energetically favored facets i.e. GB inclinations were accessible to HREM observation.

Relaxations in the form of stacking faults are incorporated into most [110] tilt GBs in Au. An example is given in Fig. 1, which shows an asymmetric GB. When the misorientation deviates from that of the low-energy (111) and (113) twins, symmetric [110] tilt GBs invariably include stacking faults that extend to one side of the GB.² In this manner the misorientation difference relative to the low-energy twins is accommodated. When the distance between stacking faults decreases to one fault for every three (111) planes, a region of the so-called 9R structure (first investigated for $\Sigma 3$ GBs in Cu³) is generated. Figure 2 shows such a GB dissociation in a $\Sigma 33$, (557)(113) Au tilt GB. Other types of GB dissociations include the formation of triangular regions bounded by two coherent and one incoherent twin in $\Sigma 9$ GBs (see Fig. 3). Whereas in this (115)(111) GB geometry the undissociated form has never been observed in Au, the planar, undissociated variety has recently been found in Al, see Fig. 4. In contrast to Au, Al has a high stacking fault energy and thus relaxations in Al do not favor the formation of stacking faults.

In spite of such structural variations that depend on the differences in interatomic interactions, considerable similarities exist among GBs in fcc materials. A common and general feature is the tendency to form well-structured GBs, with atomic structures that tend to maintain as much as possible the local atomic environment of the bulk. This often results in the formation of regions with good structural coherence, alternating with localized regions of misfit that accommodate the unavoidable structural disorder in the GB core (see Fig. 5).

References

1. D. Wolf and K. L. Merkle, in MATERIALS INTERFACES Atomic-level structure and properties, edited by D. Wolf and S. Yip (Chapman & Hall, London, 1992)87.
2. K. L. Merkle, *Interface Science* 2 (1995)311.
3. U. Wolf, F. Ernst, T. Muschik, M.W. Finnis, and H.F. Fischmeister, *Phil. Mag. A* 66 (1992)991.
4. The authors acknowledge the use of the facilities of the ANL/MSD Electron Microscopy Center. This work was supported by the U.S. Department of Energy, Basic Energy Sciences- Materials Science, under contract W-31-109-Eng-38.

Fig. 1 HREM image of $[110]$ asymmetric tilt GB in Au, misorientation $\psi = 59^\circ$.
 Fig. 2 $(557)(113)$ asymmetric tilt GB in Au: $\psi = 20.5^\circ$. Note band of 9R structure.
 Fig. 3 Triangular dissociation in $(115)(111)$ tilt GB in Au.
 Fig. 4 Planar, undissociated $(115)(111)$ GB in Al.
 Fig. 5 Misfit localizations in $(002)(111)$ GB in Au.